Sebastian Krey

HPC at GWDG

Site update and data protection on HPC systems

GWDG

Structure

- Joint data and IT-comptence center for the University of Göttingen, University clinic and the Max-Planck-Society
- Established in 1970
- Shareholders Max-Planck-Society and Unversity Göttingen, each 50%

Mission

- It is the mission of GWDG to support and enable science – now and in future – by applying appropriate technologies, developing innovative solutions, and providing reliable services
- Plan, implement and operate IT infrastructures together with/for customers

Central responsibilities

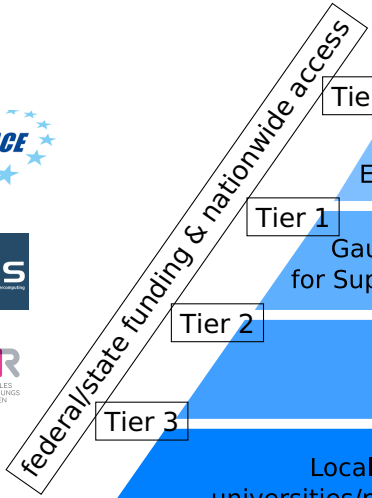
- Modern and secure IT infrastructure
- IT support for excellent research
- In-house research for innovative IT services

GWDG

Supra-regional tasks

- National High Performance Computing Center (NHR-NORD@Göttingen)
- National HPC Center of the DLR
- Upcoming regional HPC center for Lower Saxony (HPC.NDS)
- AI service center for sensitive and critical infrastructures (KISSKI)
- Partner in the AI Factory HammerHAI
- Data center in four NFDI consortia
- Host for DARIAH-EU, German National Library, GFBio, NUM CODEX, MWS, WirLernenOnline, Text+, etc.
- Cloud operator, including the Academic Cloud for universities in Germany

German HPC Infrastructure



PRACE

GCS Gauss Centre for Supercomputing

NHR NATIONALES HOCHLEISTUNGS RECHNEN

HammerHAI

KISSKI KI-Servicezentrum für sensible und kritische Infrastrukturen

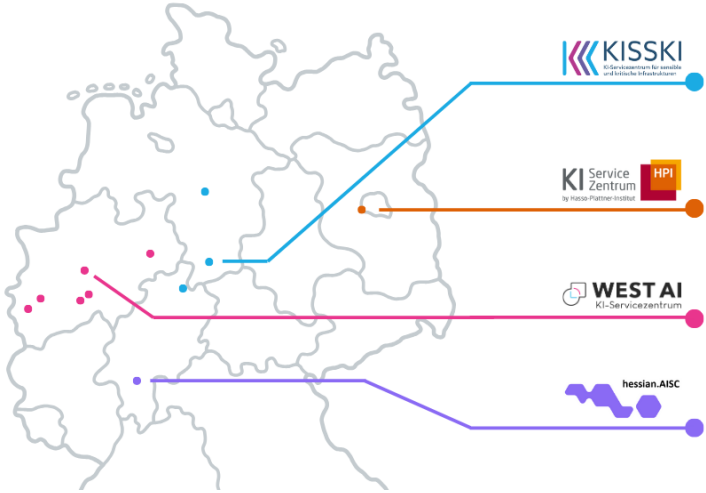
NHR-NORD@GÖTTINGEN
"Emmy", "Grete"

GWDG
Scientific
Compute
Cluster

NHR Alliance - Members

- Rhein-Westfälische Technische Hochschule Aachen
- Zuse Institute Berlin (ZIB)
- Technische Universität Darmstadt
- Technische Universität Dresden
- Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg
- GWDG/Georg-August-Universität Göttingen
- Karlsruhe Institute of Technology
- Paderborn University
- Consortium Süd-West (Goethe University Frankfurt, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Johannes Gutenberg Universität Mainz, Universität des Saarlandes)

KISSKI - ein KI-Servicezentrum für Kritische Infrastrukturen



Uni Göttingen | GWDG | CIDAS | UMG | aQua | LUH | L3S | LiFE | LUIS | MHH | Fraunhofer IEE
Sensible und kritische Infrastrukturen
Medizin & Energie

Hasso-Plattner-Institut
Bildungs- und Beratungsangebote,
Einsatz von KI in Wirtschaft &
Gesellschaft

Uni Bonn | Fraunhofer IZB | Forschungszentrum Jülich | RWTH Aachen | TU Dortmund | Uni Paderborn
KI-Hardware, KI-Beratung, KI-Schulungen sowie multimodale und transferierbare KI-Modelle

TU Darmstadt
Erklärbarkeit, Generalisierbarkeit
und kontextuelle Anpassung

Services for HPC and AI

- Infrastructure
- Scientific Software
- Consulting
- Training
- Support

One current focus is on usability, availability and security

Our Offer - AI for Everyone

- Comprehensive offering around AI
- Solutions available in browser and via API
  - ChatAI - Chatbot
- Hardware resources
  - From ARM, RISC-V to Graphcore and more
- Consulting services
- Custom development projects
- Training programs in HPC and AI
  - GWDG Academy
  - KISSKI Training Offer
  - Custom courses available upon request

CPU System “Emmy”

- Phase 1 (2018) → out of operation
  - 448 standard nodes (2 Xeon Gold 6148, 2x20 CPU-Cores, 192 GB memory)
  - High Mem nodes: 16x 768 GB
- Phase 2 (2020) → to be replaced in Q2/2026
  - 1022 standard nodes (2 Xeon Platinum 9242, 2x48 CPU cores, 384 GB memory)
  - High Mem nodes: 16x 768 GB, 2x 1,5 TB
  - 3 GPU nodes[a] (2 Xeon Gold 6148, 2x20 CPU cores, 768 GB memory, 4x NVIDIA V100)
- Since 2021 operated for the NHR alliance

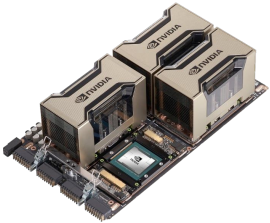
[a] The GPU nodes have been moved to Grete

CPU System “Emmy”

Add-on procurement 2022: Phase 3

- NHR NEC CPU cluster (replacement of Emmy P1)
  - 2x Intel Sapphire Rapids 8468 (48 cores) per node
  - 164x 256 GB, 164x 512 GB, 12x 1 TB, 2x 2 TB nodes
- NHR+**SCC** NEC CPU add-on 2023
  - 20+44x 512 GB, 16+4x 1 TB, 1x2 TB
  - 4 nodes per 2U chassis, each with
    - 2x Intel Sapphire Rapids 8468 (48 cores) CPU
    - 1x Cornelis Omni-Path (100 Gbit/s) HCA

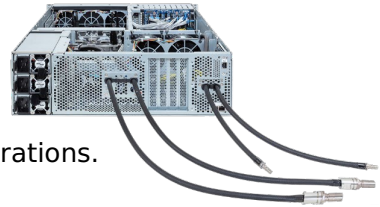
GPU System “Grete”



- Technical specification: 103+3 nodes equipped with
  - 101 MEGWARE nodes (7 racks)
    - 2x AMD Epyc 7513 CPU (32 “Milan” cores, Zen 3 microarch.)
    - 512 GB memory (DDR4, 3200 MHz)
    - 2x 1 TB NVMe SSD
    - 4x NVIDIA A100 GPU (SXM4, 80/40 GB HBM2 memory)
    - 2x Mellanox InfiniBand HCA (HDR)
  - 2 nodes with twice the cores (Zen 2 microarch.), RAM, GPUs, and VRAM
  - 3 GPU nodes moved from Emmy Phase 2
- Installed at RZGö

GPU System “Grete”

- MEGWARE GPU cluster Grete
  - Nodes from a range of projects (modular procurement):
    34x NHR, 22x REACT, 35x AI Service Center,
    9x Institutes/SFBs, 3x SCC
- MEGWARE GPU Add-on 2024
  - 25 nodes, each with
    - 2x Intel Sapphire Rapids 8468 (48 cores) CPU
    - 4x NVIDIA H100 SXM5 (94 GB) GPU
    - 2x InfiniBand HDR (200 Gbit/s) HCA
  - 3U per node, DLC
  - via RfP extension option AI Service Center
- Joint operational concept since the start of operations.



“Emmy” and “Grete” NG

Next generation 2026/2027: Phase 4

- New platform for the next CPU and GPU clusters at GWDG
- Modular procurement for NHR, SCC, HPC.NDS and KISSKI
- 350+ MEGWARE Eureka CPU nodes
- 2 installation phases
- AMD Turin and Venice CPUs (2x128 cores per node)
- 768-4096 GB memory
- 3,84 TB NVME SSDs
- Omni-Path CN5000 400G interconnect
- 15+ GPU nodes with 8xB200 Nvidia GPUs
- Reuse of CoolIT DLC infrastructure, racks and PDUs

The “Future Technology Plattform” (FTP)

- Heterogeneous hardware for development tasks
- Direct access via shell and batch system
- Offered technologies:
  - Intel Habana Gaudi 2
  - NVIDIA Grace Hopper
  - GraphCore IPU
  - Esperanto.ai
  - SpiNNaker
  - Ampere Altra
  - NVIDIA Bluefield 2
  - AMD MI300A
- Full documentation and Quick Start Guide at HPC docs
- Courses on the heterogeneous hardware at the GWDG Academy

Storage

- CephFS based HDD storage (23 PiB) successfully replaced old HDD Lustre as capacity storage
- New 1.6 PiB all-flash storage with MEGWARE supported Opensource Lustre as WORK storage at the MDC
- SSD based CephFS (0.75 PiB) well received für midrange performance applications
- VAST Data highly reliable enterprise storage with consistent low read latencies for AI
- DDN 2xES400NVX with Exa 6 and upgraded 15 TB SSD still sufficient fast main WORK storage at RZGÖ
- HSM storage succesfully migrated to new GWDG central HSM platform (currently still StorNext HSM, but probably Versity ScoutAM in the future)

Selected Challenges Mentioned by Users

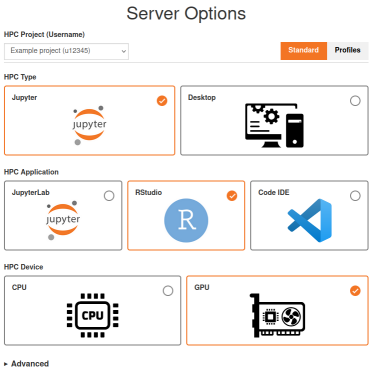
- Experience with Linux-Systems is limited
- Difficulty to debug distributed/parallel programs
- Getting access to the system
- Porting applications between centers
- Interactive access - replacing workstations
- Managing own projects, data and collaborators
- Ingress/Egress of data
- Need many concurrent users for training

Means to Lower the Bar - Usability

- Users want to do science and don’t want to become computer scientists
- Goal: Empower users to do science via
  - Tools
  - Prepared environments
  - Support
  - Consulting
  - Co-development
  - Training
  - Community
- Data management, data exploitation is part of science, too!

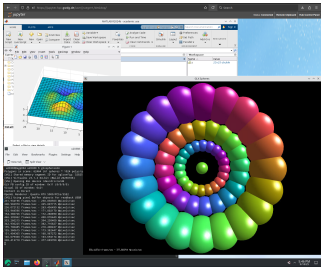
JupyterHPC

- Quick and easy way to access HPC resources via
  - No ssh setup necessary
  - Frictionless and comfortable even for beginners
  - Very useful for courses, trainings and fallback fo
- CPU and GPU nodes available
- Classic Jupyter notebooks with various kernels
  - Python, Julia, R, Bash, SageMath
- All container recipes open source
  - Easy to build and run your own containers



HPC Desktops

- Goal: own HPC-powered workstation
- Integrated with Jupyter HPC
- Fully featured Linux desktops via webVNC
  - KDE, Gnome, XFCE available
- Fully hardware accelerated rendering on GPU nodes
  - Performant software rendering via llvmpipe on CPU nodes
- Complete HPC environment accessible
  - Regular module system, same as in standard ssh sessions
  - Documentation applies unchanged
  - Possible to start Slurm jobs from desktop sessions



Data protection and security

- Secure HPC environment for batch processing of medical data
- Workflow adapted for other types of critical data
- Further improvements to simplify deployment and scale out in development
- Certification of processing data of highest non-classified data protection levels in preparation
- All OS image and configuration changes only with signed Git commits
- Critical backend system administration only by dedicated priviledged admin workstations (PAW)
- Central logfile protection against manipulation
- Next step: Securing HPC deployment with Secure Boot (mostly done)

Secure Boot

- Opensource deployment tool Warewulf
- Communication with Warewulf SSL secured
- Signed secure boot enabled iPXE bootloader
- Signed custom kernel modules with own custom key
- Deployed custom key to BIOS of all user accessible nodes
- Only one hardware plattform did not work (soon to be phased out)

What are privileged admin workstation

- Terminology from the Microsoft world
- Centrally managed devices for administration of critical infrastructure
- Maximize privilege separation (admin account of PAW has no admin privileges on the critical infrastructure and vice versa)
- Dedicated network segment (VPN profile)
- Restricted network access (no internet access)
- Restricted software availability (only tools necessary for the task)
- Logging of configuration changes and software installations

Why and for what use PAW?

- In MS world: All tasks requiring domain admin privileges (root on all nodes of the domain)
- Jumphost for external admin access
- Central logserver
- Key management systems
- Build infrastructure for OS images
- Network management

What is required and desired for setting up a PAW?

- Required
  - Automated deployment and configuration of PAW
  - Monitoring of configuration and software installations on the PAW
  - Central logging and analysis infrastructure for monitoring data
  - Network or VPN profiles for accessing only the critical infrastructure via PAW
  - Automated user setup
- Desired
  - No complicated device management infrastructure
  - Personalized work environment on PAW should be possible
  - Software installation from white listed pool

GWDG HPC PAW solution

- Management:
  - Mainly based on Fedora and Kickstart
  - Installation ISO and repo config from trusted mirror
  - All configurations in internal Git repository
  - Git repository requires signed commits
  - List of approved keys for signature also in Git
- Configuration
  - UEFI Secure boot
  - Systemd-boot without kernel commandline editor
  - `root` account locked, LUKS, preconfigured `sudo`, `firewalld`, etc.
  - Removal of remote management tools (SSH server, cockpit, etc.)
  - `pam-u2f` for 2FA
  - User setup includes eduroam and eduVPN setup
  - Shell script for software installation kiosk
  - Shell script with systemd timer for monitoring

PAW logging infrastructure

- Graylog based
- Daily Systemd timer executes monitoring script and creates JSON
- Logging of Laptop type, Serial number, BIOS information
- `rkhunter` results
- All software packages with version (package manager and flatpaks)
- All executeables with set SUID, SGID or capabilities

Why WORM logs?

Processing risk class D information (e.g. medical data) requires auditable access logs. This means:

- Central log aggregation
- Verifiable integrity
- Redundant long term storage
- Prevent changes to log files
- No deletion from a single person

How to solve the requirements?

Central: Redirect Journald to Rsyslog, send Rsyslog to central server, individual files for each server

Integrity: Daily logfiles, create checksums

Redundant storage: Offsite backups (incl. checksums) on tape

Deletion prevention : `root` is god $\rightarrow$ difficult (can even change SELinux settings)

File modificationdeletion prevention

Modificationdeletion prevention from normal users easy:

- Extended attributes `append-only` and `immutable`
- Creating new log files with apppend`-only` prevents deletion of older log entries
- Adding `immutable` attribute at the end of the day (before checksum creation) to prevent deletion
- Integrity check of scripts handling these operations with checksums

Superuser `root` still has permission to remove these extended attributes
$\rightarrow$ can modify or delete files and hide it by creating new checksums.

Further integrity enhancing measurements

Securing remote `root` logins:

- Changing the append-only and immutable attributes require `CAP_LINUX_IMMUTABLE`
- Removing this capability from sshd via (immutable) service override
  $\rightarrow$ `root` via SSH has lost the permission to change append-only and immutable attribute
- Remote administration via SSH still possible
- Prevent usage of IPMI remote and serial console, e.g. no network connection
- Prevent local IPMI usage/configuration change by disabling OS access to BMC (BIOS setting)

Further integrity enhancing measurements

Securing local accesss:

- Server location in accesss restricted area of data center
- Persons with access to data center area must not know password for root or sudo enabled user accounts
- Persons with local login permissions must not have permission to access the restricted data center area alone
- Additionally require 2FA for local login (e.g. FIDO Key via pam-u2f)

Trusted Research Environments (TREs)

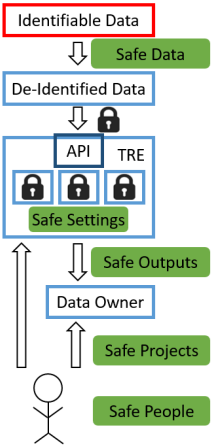
- TREs provide **highly secure** environments for analyzing sensitive data
- All computations and analysis are conducted entirely within the TRE
  - Results are manually reviewed pre-publication
- Based on the "5 SAFE" framework from the UK Office of National Statistics
- Also known as:
  - **Secure Processing Environments (SPEs)** (Common in DE/EU)
  - Secure Data Environment (SDE) (Common in England; Especially NHS)
  - Data Safe Havens (Common in UK; Especially Scotland)

Other Reasons for a TRE

- **Reprocucibility**
  - Controlled Environments
  - Container-Images are publishable
- **HPC-Resources (incl. GPU-Access)**
  - Big Data, for example Genome Analysis
  - Machine-Learning Models
- **Outsourcing and Centralizing Security/Administration Burden**
- **Legislative Pressure**
  - Europe: European Health Data Space
  - Germany: Gesundheitsdatennnutzungsgesetz

5 Safes

1. Safe People
   - Trustworthy institutions and “Know your Customer”
   - Completed training, Signed user agreement
2. Safe Projects
   - No access without data owner’s approval
3. Safe Settings
   - Data is only processed within the TRE
   - No internet access, no download possible
4. Safe Outputs
   - Manual approval of exports before publication
   - Focus: No re-identification; Only aggregated data
5. Safe Data
   - Data is pseudonymized when ingested into the TRE



On-Premise HPC-based TRE: GöTRE

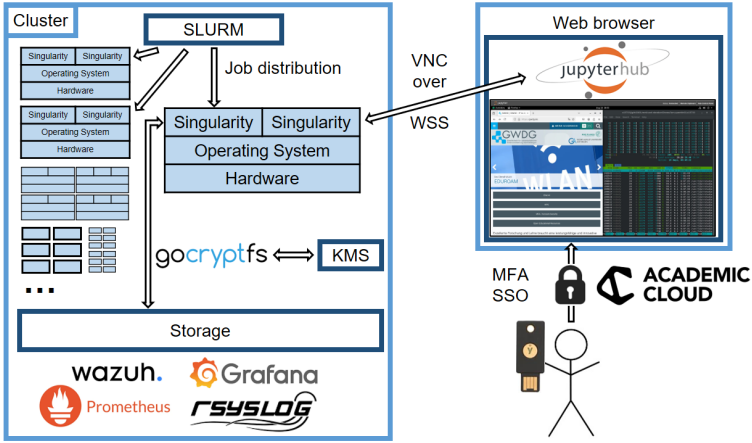
Technical Features

- Zero-Trust Architecture
- End-to-End Encryption on file system level
  - Transparent to the user
- Multi-Factor Authentication
- Collaborative Work possible
  - Analogous to Windows Fileserver
- Complete Audit-Log
- One Key per File
  - Secure Sharing via Key Management System

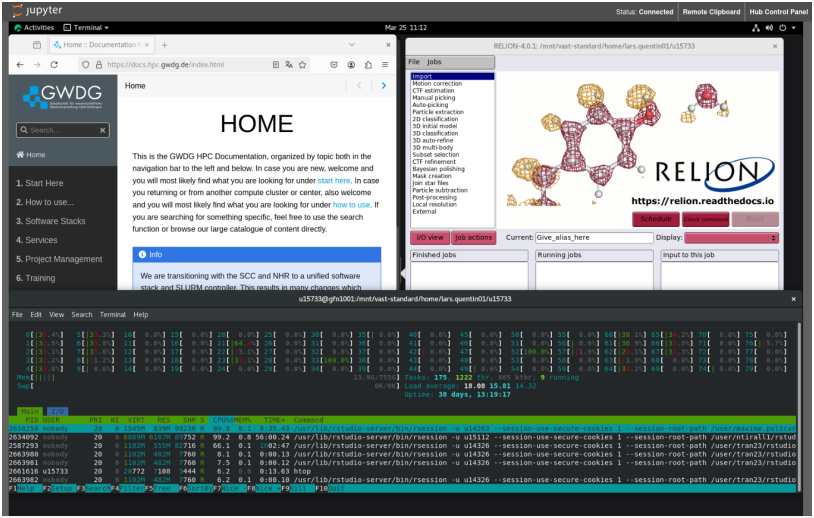
Organizational Features

- *High Usability* despite *Strong Security*
  - Access via web interface
  - No client software required
  - Graphical desktop environment
  - Supports non-web-based applications
- Embedded in HPC Infrastructure
  - High Performance
  - Machine-Learning support via GPUs

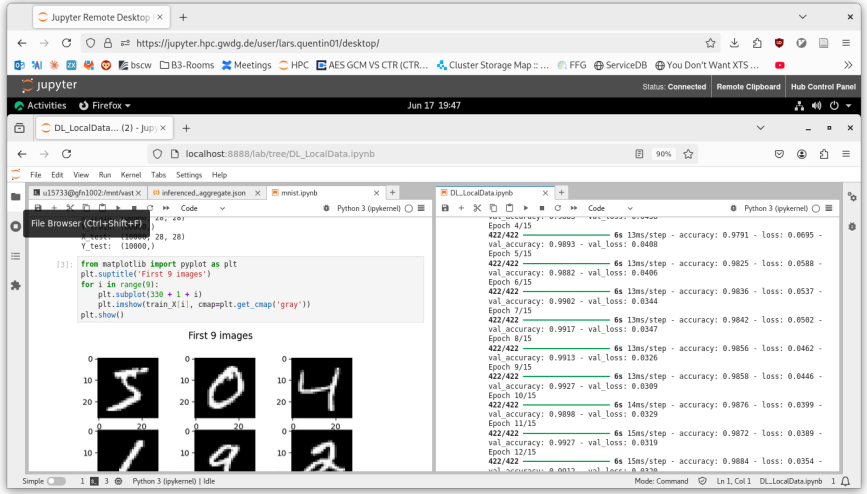
GöTRE: Architecture



GöTRE: Interface



GöTRE: Interface



Outline

Summary

- GWDG offers various HPC resources
- There are many ways to get access
- Besides performance, usability and availability can matter
- Providing highest data protection standards important esp. for medical research
- Combination of data protection and good usability possible